New Estimates On Various Critical/Universal Quantities
of the 3D Ising Model [*]

M. Hasenbusch[a] and K. Pinn[b]

[a]Fachbereich Physik, Humboldt-Universität zu Berlin,
Invalidenstr. 110, D-10099 Berlin, Germany

[b]Institut für Theoretische Physik I, Universität Münster,
Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany

We present estimates for the 3D Ising model on the cubic lattice, both regarding interface and bulk properties. We have results for the interface tension, in particular the amplitude σ_0 in the critical law $\sigma = \sigma_0\, t^\mu$, and for the universal combination $R_- = \sigma\, \xi^2$. Concerning the bulk properties, we estimate the specific heat universal amplitude ratio A_+/A_-, together with the exponent α, the nonsingular background of energy and specific heat at criticality, together with the exponent ν. There are also results for the universal combination $f_s\, \xi^3$, where f_s is the singular part of the free energy. Details can be found in [1] (interface) and [2] (bulk).

1. INTRODUCTION

In this conference contribution, we summarize recent efforts [1,2] to determine various critical quantities of the 3D Ising universality class using the Monte Carlo (MC) method. These efforts are worthwhile for at least three reasons: 1) There are many systems in nature belonging to the Ising universality class. Thus a comparison of theoretical predictions with experimental results is possible. 2) Getting precise estimates is still a challenge, both from the algorithmic side and from a theoretical point of view. MC data with increasing statistical precision put standard assumptions to test and may require more and more refined theoretical modelling. 3) MC precision has now become competitive with, e.g., high/low temperature series expansions, the ϵ-expansion and 3D field theoretic calculations. Comparing the results is interesting and might point out sources of systematic errors in either method.
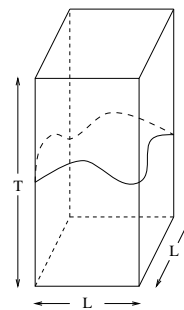
2. INTERFACE PROPERTIES

Properties of interfaces separating extended domains of different phases are of great interest,

both from the experimental and the theoretical point of view. For recent experimental work measuring observables that are related to and can be compared with quantities studied in the present work, see [3,1].

Figure 1
Lattice geometry

We consider the 3D Ising model on a cubic lattice of size $L \times L \times T$ with spins $s_x = \pm 1$, Hamiltonian $H(s) = -\beta \sum_{<x,y>} s_x s_y$, where $<xy>$ denotes a pair of nearest neighbour sites on the lattice, and partition function $Z = \sum_s \exp[-H(s)]$. By Z_p we denote the partition function with periodic boundary conditions in all three directions. Antiperiodic boundary conditions in t-direction favour the occurence of interfaces (perpendicular

to the t-axis), see figure 1. The corresponding partition function is denoted by Z_a. If we can assume that there is exactly one interface in the system, its free energy is given by

$$F_s = F_a - F_p + \ln T, \tag{1}$$

where $\ln T$ takes care of the free motion of the interface in the t-direction.

We obtained the interface free energies by integration of the interface energy $E_s = \langle H \rangle_a - \langle H \rangle_p$:

$$F_s = F_s(\beta_o) + \int_{\beta_o}^{\beta} d\beta' \, E_s(\beta'). \tag{2}$$

Various state of the art algorithms were employed: the boundary flip cluster algorithm for the determination of $F_s(\beta_0)$, the Wolff single cluster, the Ising interface cluster and the multispin coded demon algorithm for the determination of E_s. Detailed descriptions and the appropriate references can be found in [1].

Interface tensions σ were then obtained by fitting the free energies with either

$$F_s \simeq C_s + \sigma L^2 \tag{3}$$

or [4]

$$F_s \simeq C_s + \sigma L^2 + 1/(4\sigma L^2). \tag{4}$$

We chose lattice sizes 32^3, 48^3, 64^3 and 96^3. Data were taken on a dense grid of β values in the range $0.223 \dots 0.23$. In table 1 we quote a few of our fit results for the interface tension. Here, "fit2" la-

Table 1
Selection of σ estimates

fit	$\beta = 0.2240$	$\beta = 0.2255$
fit2	0.004784(9)	0.008810(9)
96vs64	0.004799(17)	0.008822(18)
fit3	0.004782(6)	0.008801(6)

bels a fit with eq. (3), discarding the $L = 32$ data, under the name of "96vs64" goes a determination of C_s and σ from the $L = 64$ and $L = 96$ data alone, and "fit3" refers to a fit of data from all four lattice sizes with eq. (4). The results from the different fit types are fairly consistent.

Our next task was to fit the interface tension results to the critical law

$$\sigma(\beta) \simeq \sigma_0 \, t^\mu (1 + a_\theta t^\theta + a_1 \, t). \tag{5}$$

Here we included the leading corrections to scaling terms. We compared the results stemming from the two definitions of the reduced temperature, $t_1 = \beta/\beta_c - 1$ and $t_2 = 1 - \beta_c/\beta$. Furthermore, we fixed the following parameters: $\beta_c = 0.2216544(6)$ [5], $\mu = 1.262$, and $\theta = 0.51$ [5]. These were the most precise estimates we could find in the literature. The fit results are quoted in table 2, again for three different fit schemes.

Table 2
Fit results for σ_0, a_θ and a_1

fit	t-def	σ_0	a_θ	a_1
fit2	t_1	1.549(11)	-0.409(72)	0.01(20)
	t_2	1.549(11)	-0.397(76)	1.13(21)
fit3	t_1	1.5428(73)	-0.376(49)	-0.06(14)
	t_2	1.5421(73)	-0.362(51)	1.06(14)
96vs64	t_1	1.571(20)	-0.57(13)	0.47(36)
	t_2	1.571(21)	-0.56(13)	1.61(37)

Note that the σ_0 results for the two $t-$definitions are always consistent with each other. a_1 should have a jump of $\mu \approx 1.26$ which is obeyed within the errors. Taking into account the various sources of uncertainty (including the variation with the type of fit) we arrive at the final estimate $\sigma_0 = 1.55(5)$.

We finally employed our σ-data in an estimation of the universal ratio R_-. Including corrections to scaling, it can be defined through

$$R_- = \sigma(\beta)\,\xi(\beta)^2 - c\,\xi^{-\omega}, \tag{6}$$

where $\beta \to \beta_c$ from above. ω is the correction to scaling exponent. We fixed it to $0.81(5)$ [5]. The ξ-data were taken from [6]. Our result is $R_- = 0.1040(8)$, where the error is mainly due to the uncertainty in the exponent ω. A comparison with some results from the literature is given in [1].

3. BULK PROPERTIES

We consider a 3D Ising model on a cubic lattice of size L^3, with periodic boundary conditions in all three directions. Important quantities are the free energy per volume

$$f = -1/(3\,L^3)\ln Z\,, \qquad (7)$$

the energy, $E = -df/d\beta$ and the specific heat, $C = dE/d\beta$. The quantities are split in a non-singular and a singular part, e.g., $E = E_{ns} + E_s$. By standard arguments the following finite size scaling laws are expected to hold:

$$
\begin{aligned}
E &\simeq E_{ns} + const_E\, L^{-d+1/\nu} \\
C &\simeq C_{ns} + const_C\, L^{-d+2/\nu}
\end{aligned}
\qquad (8)
$$

at criticality, and

$$E \simeq E_{ns} - C_{ns}\,\beta_c\, t \mp A_\pm\, \beta_c\, \frac{|t|^{1-\alpha}}{1-\alpha}\,, \qquad (9)$$

above and below the transition. Using state of the art algorithms we obtained estimates for energy and specific heat at $\beta_c = 0.2216544$ for L ranging from 12 to 112. The relative error of the energy is of order 10^{-5} throughout. We then did a combined fit of energy and specific heat to eq. (8). Our results for ν, E_{ns} and C_{ns} are given in table 3. L_{min} is the smallest lattice size used for

Table 3
Fit results from critical energy and specific heat

L_{min}	X	ν	E_{ns}	C_{ns}
12	5.6	0.6316(4)	0.330229(5)	-12.13(33)
16	2.25	0.6315(8)	0.330218(7)	-11.83(61)
20	0.75	0.6308(10)	0.330209(8)	-11.12(76)

the fit, and X denotes χ^2 per degree of freedom. We find the precision of the ν-estimate of the last line of the table quite remarkable.

In the off critical case, we always aimed at the infinite volume limit of the energy. Our data cover the range from $\beta = 0.21971$ to $\beta = 0.2230$. Lattice sizes up to $L = 128$ were employed. The results of fits with eq. (9) are given in table 4. Again we used two definitions of t, namely

Table 4
Fit results from off critical energy

	t_1	t_2
α	0.1115(37)	0.1047(48)
A_+/A_-	0.550(12)	0.567(16)
E_{ns}	0.33029(3)	0.33030(4)
C_{ns}	-9.86(80)	-11.37(1.17)

$t_1 = 1-\beta/\beta_c$ and $t_2 = \beta_c/\beta - 1$. There is a slight mismatch of the estimate for E_{ns} with the estimates from the critical data in table 3. It is most likely due to corrections to scaling that have not been taken into account.

We finally estimated the universal constant $f_s\,\xi^3$ on both sides of the transition. Estimates for f_s were obtained by integration over β of the singular part of the energy, obtained from the approximation $E_s \approx E - E_{ns} - C_{ns}(\beta - \beta_c)$. Using our background estimates E_{ns} and C_{ns} together with the correlation lengths given in [6], we obtained $f_s\,\xi^3 = 0.0355(15)$ for $\beta \nearrow \beta_c$, and $f_s\,\xi^3 = 0.0085(2)$ for $\beta \searrow \beta_c$.

4. CONCLUSIONS

For various interface and bulk quantities we could significantly improve on older numerical estimates. Especially interesting is the quite precise determination of ν from the finite size scaling of the energy and specific heat at criticality.

REFERENCES

1. M. Hasenbusch and K. Pinn, cond-mat/9704075, to appear in Physica A.
2. M. Hasenbusch and K. Pinn, cond-mat/9706003.
3. T. Mainzer and D. Woermann, Physica A 225 (1996) 312.
4. M. Caselle et al., Nucl. Phys. B 432 (1994) 590, and references therein.
5. A.L. Talapov and H.W.J. Blöte, J. Phys. A 29 (1996) 5727.
6. M. Caselle and M. Hasenbusch, J. Phys. A 30 (1997) 4963.